I U C L I D

D at a S e t

Existing Chemical	ID: 3173-53-3
CAS No.	3173-53-3
EINECS Name	cyclohexyl isocyanate
EINECS No.	221-639-3
Molecular Formula	C7H11NO
Molecular Weight	125.17
Producer Related Part	
Company:	Bayer Corporation
Creation date:	15-JUL-1999
Substance Related Part	
Company:	Bayer Corporation
Creation date:	15-JUL-1999
Memo:	Bayer Corporation
Printing date:	23-APR-2001
Revision date:	
Date of last Update:	23-APR-2001
Number of Pages:	9
Chapter (profile) :	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8, 5.9
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile) :	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 Melting Point

Value: -80 degree C
Method: other: historical data
Testsubstance: other TS: cyclohexylisocyanate
Flag: Critical study for SIDS endpoint
23-APR-2001 (1)

2.2 Boiling Point

Value: 172 degree C at 1013 hPa
Method: other: Handbook value
Testsubstance: other TS: cyclohexylisocyanate; purity not noted
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
20-APR-2001 (2)

2.4 Vapour Pressure

Value: 2.2 hPa at 20 degree C
Method: other (measured): historical data
Testsubstance: other TS: cyclohexylisocyanate
Flag: Critical study for SIDS endpoint
23-APR-2001 (1)

Value: 12 hPa at 50 degree C
Method: other (measured) : historical data
Testsubstance: other TS: cyclohexylisocyanate
Flag: Critical study for SIDS endpoint
23-APR-2001 (1)

2.5 Partition Coefficient

log Pow:
Method:
Year:
Testsubstance: other TS: cyclohexylisocyanate
Remark: A log Pow is not determinable due to the instability in water.
Flag: Critical study for SIDS endpoint
23-APR-2001 (1)

2.6.1 Water Solubility

Qualitative: other: rapid hydrolysis
Testsubstance: other TS: cyclohexylisocyanate
Flag: Critical study for SIDS endpoint
23-APR-2001 (1)

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1560000 molecule/cm3
Rate constant: .00000000001 cm3/(molecule * sec)
Degradation: 50 % after 12.8 hour(s)
Method: other (calculated): AOP Program (v1.89)
Year: GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
23-APR-2001 (3)

3.1.2 Stability in Water

Type :
Method:
Year: GLP:
Test substance:
Remark: Hydrolysis !
Flag: Critical study for SIDS endpoint
23-APR-2001 (1)

3.3.1 Transport between Environmental Compartments

Type : fugacity model level III
Media: other: air, water, soil, sediment
Air (Level I):
Water (Level I) :
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: EPIWIN Level III Fugacity Model
Year: 1999
Result:

	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	7.03	25.7	1000	8.77e-011
Water	31	360	1000	1.33e-008
Soil	61.6	360	1000	2.53e-008
Sediment	0.365	1.44e+003	0	6.37e-009

Persistence Time: 213 hr
Reaction Time: 272 hr
Advection Time: 987 hr
Percent Reacted: 78.4
Percent Advected: 21.6
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
23-APR-2001 (3)

3.5 Biodegradation

Type :	aerobic
Inoculum:	predominantly domestic sewage
Concentration:	.8 mg/l
Degradation:	75 % after 20 day
Method:	OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year:	1979 GLP: no
Test substance:	other TS: purity: approx. 98 %
Remark:	1 g/l Emulgator W (CAS-No. 68130-72-3) used as emulsifier
Reliability:	(2) valid with restrictions
Flag:	Critical study for SIDS endpoint

23-APR-2001 (1)

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type:	static
Species:	Leuciscus idus (Fish, fresh water)
Exposure period:	72 hour(s)
Unit:	mg/l Analytical monitoring: no
LC0:	.5
Method:	other: Bestimmung der Wirkung von Wasserinhaltsstoffen auf Fische. DEV, L 15 (1979)
Year:	1979 GLP: no
Test substance:	other TS: purity: approx. 98 %
Remark:	range finding test
Flag:	Critical study for SIDS endpoint

23-APR-2001 (1)

4.2 Acute Toxicity to Aquatic Invertebrates

4.3 Toxicity to Aquatic Plants e.g. Algae

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type:	LD50
Species:	rat
Strain:	Sprague-Dawley
Sex:	male/female
Number of Animals:	20
Vehicle:	other: undiluted
Value:	560 mg/kg bw
Method:	
Year:	1974 GLP: no data
Test substance:	other TS: cyclohexyl isocyanate; purity not noted
Method:	The undiluted compound was fed by stomach tube to Sprague-Dawley albino male and female rats. After the approximate Minimal Lethal Dose was determined, groups of male and female rats were fed in increasing doses at increments of 0.1 fractional log intervals at four levels to cover the toxicity range. The data was used to calculate LD50 by the method of EJ de Beer. Observations were made for toxic signs over a 14 day period and the viscera of the animals were examined macroscopically.
Result:	The single oral dose LD50 for male and female rats was placed at 560mg/kg bw with lower and upper limits of 490 to 630 mg/kg bw. Toxic signs included reduced appetite and activity (1-3 days in survivors), increasing weakness, collapse, and death. Survival time was several hours to 2 days. Autopsy findings were lung and liver hyperemia, and acute gastrointestinal inflammation. Surviving animals were sacrificed 14 days afer dosing. The viscera appeared normal by macroscopic examination.
Reliability:	(2) valid with restrictions
Flag:	Critical study for SIDS endpoint

23-APR-2001 (4)

Type:	LD50
Species:	rat
Strain:	Sprague-Dawley
Sex :	male/female
Number of Animals:	4
Vehicle:	other: 20% ethanol-80% propylene glycol solution
Value:	335 - 625 mg/kg bw
Method:	other
Year:	1974 GLP: no data
Test substance:	other TS: cyclohexyl isocyanate; purity = technical grade
Method:	Male Sprague-Dawley rats (weighing 270-300g) and females (weighing 200-250g) were fasted for 24 hours before the compound was administered. The compound was diluted so that each animal received its dose in a volume equivalent to 0.1-0.2% body weight. Graded doses were given to four groups of 4 animals by gavage. Symptoms and mortality were recorded for 14 days and the LD50 calculated by the method

	of Weil (CS Weil, 1952. Biometrics. 8:349).
Result:	LD50 = 625 mg/kg bw (females) LD 50 = 335 mg/kg bw (males)
	Rats exhibited symptoms of lethargy and, depending on dose, proceeded to profound sedation.
Reliability:	(2) valid with restrictions
Flag:	Critical study for SIDS endpoint

23-APR-2001 (5)

5.1.2 Acute Inhalation Toxicity

Type :	LC100
Species :	rat
Strain:	
Sex:	male
Number of Animals:	6
Vehicle:	other: undiluted
Exposure time:	2.5 hour(s)
Value:	ca. 7160 mg/m³
Method:	
Year:	GLP: no data
Test substance:	other TS: cyclohexyl isocyanate; purity not noted
Method:	Six mature male rats were placed in a stainless steel chamber of 35 liter capacity and exposed to a concentrated atmosphere of vapors produced by passing a stream of air through 42.4g of the compound contained in a 500ml Erlenmeyer flask. Vapors from the flask were passed though a one liter bottle to remove droplets and then into the chamber. Air flow through the chamber was 4.0 liter/min as measured by a calibrated rotameter. No supplementary air was introduced. The animals were observed for behavior until all succumbed. The viscera of the animals was examined macroscopically.
Result:	All six animals succumbed within 2.5 hours after start of exposure. Ocular discharge, labored breathing, and slight lethargy were observed during the first hour of exposure. During l-2.5 hours of exposure, the animals exhibited increased weakness, collapse and death. Hemorrhagic lungs were seen upon autopsy. Average concentration of the vapors in the chamber was calculated to be 7.16g/m3 (1393 ppm).
Reliability:	(2) valid with restrictions
Flag:	Critical study for SIDS endpoint

23-APR-2001 (4)

Type:	LC100
Species:	rat
Strain:	
Sex:	male/female
Number of Animals:	8
Vehicle:	other: undiluted
Exposure time:	2 hour(s)
Value:	ca. 13523.76 mg/m³
Method:	
Year:	GLP: no data
Test substance:	other TS: cyclohexyl isocyanate; purity = technical grade
Method:	The rats were supported on a wire mesh rack inside a 20 liter chamber equipped with a window and exposed to an atmosphere saturated with the test substance. Vapors were generated by passing a stream of air over a known quantity of test material. The air flow was measured by a calibrated flowmeter. Animals were observed until both succumbed.
Result:	Exposure of rats to a saturated vapor of the compound caused noticable eye irritation, dyspnea, salivation, piloerection, and death to all animals exposed. Death occurred within 2 hours. Calculated exposure concentration was approximately 2631.5 ppm (13523.76 mg/m3).
Reliability:	(2) valid with restrictions
Flag:	Critical study for SIDS endpoint
23-APR-2001	(5)

5.1.3 Acute Dermal Toxicity

Type :	other: MLD
Species:	rabbit
Strain:	
Sex:	male/female
Number of Animals:	5
Vehicle:	other: undiluted
Value:	2000 - 3160 mg/kg bw
Method:	
Year:	GLP: no data
Test substance:	other TS: cyclohexyl isocyanate; purity not noted
Method:	The undiluted compound was applied in increasing doses at increments of 0.2 fractional log intervals to the closely clipped, intact skin of New Zealand albino male and female rabbits. The treated areas were covered with plastic strips and the animals held in wooden stocks for periods up to 24 hours, after which they were assigned to individual cages. Observations were made for toxic signs over a 14 day period and the viscera of the test animals were examined macroscopically.
Result:	The acute skin absorption Minimal Lethal Dose for male and female rabbits was found to be greater than 2000 and less than 3160 mg/kg bw. Toxic signs included reduced appetite and activity (2-4 days in the survivors), increasing weakness, collapse and death. Survival at the higher doses

was less than 24 hours. Autopsy findings were hemorrhagic lungs, slight liver discloration and gastrointestinal inflammation. Surviving animals were sacrificed 14 days after dosing. The viscera appeared normal by macroscopic examination.

Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
23-APR-2001 (4)

Type : other: MLD
Species: rabbit
Strain:
Sex : male/female
Number of Animals: 4
Vehicle: other: undiluted
Value: 500 mg/kg bw
Method: other
Year: 1974 GLP: no data
Test substance other TS: cyclohexyl isocyanate; purity = technical grade
Method: Male and female New Zealand white rabbits (weighing 2-3 kg) were exposed to undiluted compound on their shaved backs for 24 hours, after which the compound was removed. Doses were 200, 500, 1000, 2000 mg/kg bw. Symptoms and mortality were recorded for 14 days.
Result: Minimal Lethal Dose = 500 mg/kg bw
The only obvious symptom was tachypnea.
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
23-APR-2001 (5)

5.1.4 Acute Toxicity, other Routes

5.4 Repeated Dose Toxicity

5.5 Genetic Toxicity 'in Vitro'

5.6 Genetic Toxicity 'in Vivo'

5.8 Toxicity to Reproduction

5.9 Developmental Toxicity/Teratogenicity

(1) Bayer AG data

(2) CRC Handbook of Chemistry and Physics. 80th edition (1999-2000) David R. Lide, ed. CRC Press, New York. p 3-123 No. 4416.

(3) Meylan W. and Howard P. (1999) EPIWin Modeling Program. Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510.

(4) Younger Laboratories Study # 9495YLR74 (unpublished)

(5) Chemagro Study #40870 (unpublished)